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Gas Chromatography/Matrix Isolation-Infrared Spectrometry for the Identification of Polycyclic Aromatic Hydrocarbons in Urban Air Particulate Matter

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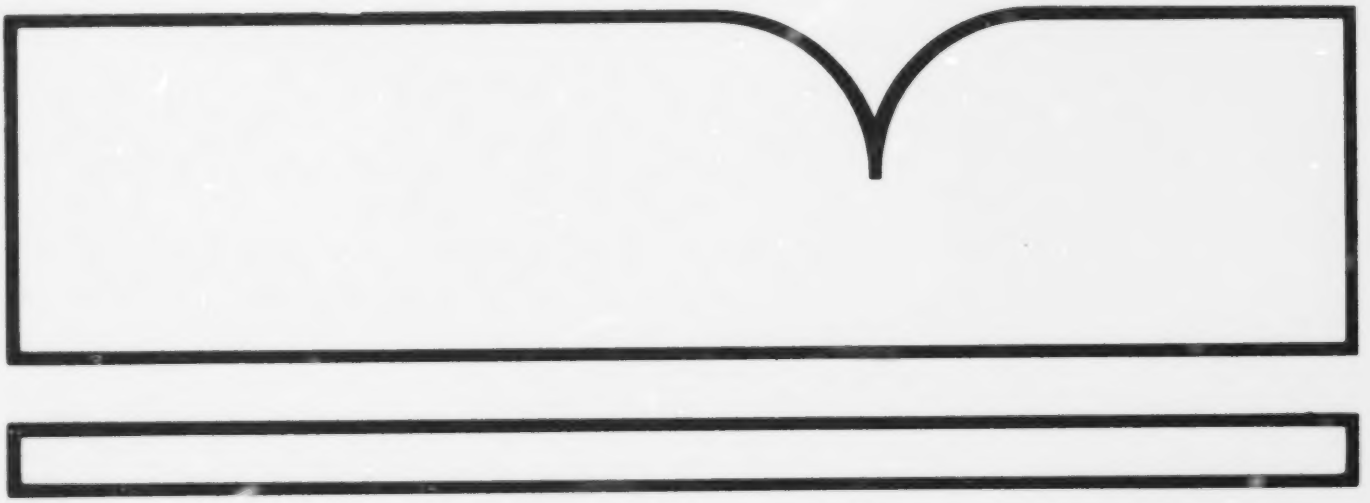

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16. ABSTRACT

The capabilities of gas chromatography/matrix isolation-Fourier transform infrared (GC/MI-FTIR) spectrometry for detecting and identifying polycyclic aromatic hydrocarbons (PAHs) in urban air particulate matter are demonstrated. The ability of GC/MI-FTIR to discriminate between PAH isomers that are difficult to distinguish by gas chromatography/mass spectrometry is shown. The MI-FTIR spectra of PAHs obtained under GC/MI-FTIR conditions are comparable to those reported in the literature that were obtained by conventional MI-FTIR techniques.

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Gas Chromatography/Matrix Isolation-Infrared Spectrometry for the Identification of Polycyclic Aromatic Hydrocarbons in Urban Air Particulate Matter*

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The capabilities of gas chromatography/matrix isolation-infrared (GC/MI-IR) spectrometry for detecting and identifying polycyclic aromatic hydrocarbons (PAHs) in urban air particulate matter are demonstrated. The ability of GC/MI-IR to discriminate between PAH isomers that are difficult to distinguish by conventional electron-impact ionization gas chromatography/mass spectrometry is shown. The MI-IR spectra of PAHs obtained under GC/MI-IR conditions are comparable to those reported in the literature that were obtained by using slow-spray-on matrix deposition techniques.

Index Headings: **Polycyclic aromatic hydrocarbons; Gas chromatography/matrix isolation-infrared spectrometry.**

INTRODUCTION

Polycyclic aromatic hydrocarbons (PAHs) constitute a significant fraction of airborne particulate matter. Although some PAHs occur naturally, many PAHs in the environment are formed by the incomplete combustion of fossil fuels and other organic materials. Several sources of PAHs, such as coal-fired power plants, automobile and diesel exhaust, and residential wood-stoves and fireplaces, have been identified.[1,2] There is considerable interest in the characterization of PAHs in the environment because many of these compounds exhibit carcinogenicity in laboratory test animals or mutagenicity in bacteria.[3,4]

Analyses for PAHs are difficult because many of the isomers cannot be separated by gas chromatography (GC) or easily distinguished by electron-impact ionization (EI) gas chromatography/mass spectrometry (GC/MS). The ability to discriminate between PAH isomers in environmental samples is crucial in assessing the associated health risks because PAH isomers often exhibit vastly different biological activities, such as the degree of carcinogenicity or mutagenicity.[3,4] Gas chromatography/infrared (GC/IR) spectrometry is a powerful technique for isomer discrimination, but its use in PAH analyses has been limited historically by poor sensitivity. Although low-nanogram sensitivity for strongly IR absorbing and environmentally important compounds, such as esters, aryl ethers, and N-nitrosoamines, has been reported for light-pipe-based, on-the-fly GC/IR systems, identification limits for PAHs were 50 ng or greater.[5] Analyzing PAHs by on-the-fly GC/IR is difficult because of their relatively weak IR absorbances and high boiling points, which may lead to broad, late-eluting GC peaks that produce IR spectra with poor signal-to-noise ratios. An alternative to on-the-fly GC/IR uses matrix isolation (MI) to trap the GC eluites for subsequent IR spectral analysis.

The combination of MI and IR spectrometry for characterizing PAHs first incorporated Knudsen effusion to prepare the matrix-isolated samples.[6] This enabled submilligram quantities of solid PAHs to be analyzed and up to 10 co-deposited PAHs to be identified.[7] In other studies using MI-IR spectrometry, four of the six monomethylchrysene isomers[8] and several isomeric methylnaphthalenes and methylbiphenyls[9] were distinguished. Variable-temperature vacuum sublimation was also used to achieve limited fractionation of PAH-containing mixtures during sample deposition.[10] These experiments led to the combination of GC and MI-IR spectrometry for characterizing PAHs in solvent-refined coal and coal-derived crude oil.[11]

In a parallel development, a GC/MI-IR system was designed and constructed in which the GC effluent is deposited in a continuous matrix on a rotating, mirror-surfaced cylinder.[12] A commercial instrument based on this prototype was introduced in 1984.[13] Several applications of GC/MI-IR spectrometry have been reported in the literature.[14] Current efforts in our laboratory involve the development and evaluation of GC/MI-IR spectrometry for characterizing organic compounds in complex environmental samples. Preliminary results from our laboratory have illustrated the potential of GC/MI-IR spectrometry for detecting and identifying PAHs in environmental air sample extracts.[15-17] Here, we describe the use of GC/MI-IR spectrometry for identifying specific PAH isomers in an extract from urban air particulate matter.

EXPERIMENTAL

All GC/MI-IR data were collected on a Mattson Instruments (Madison, WI) Cryolect system.[18] The Cryolect system consists of a Mattson Instruments Sirius

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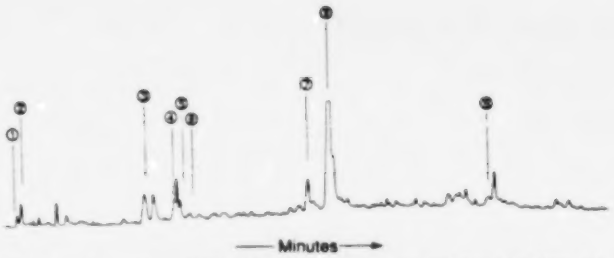

FIG. 1. A portion of the GC/FID trace for an extract of urban air particulate matter collected on a quartz-fiber filter. Peak identification: (1) benz[*a*]anthracene, 31.24 min; (2) chrysene and triphenylene, 31.58 min; (3) benzofluoranthenes, 41.28 min; (4) benzo[*e*]pyrene, 43.61 min; (5) benzo[*a*]pyrene, 44.03 min; (6) perylene, 44.79 min; (7) indeno[1,2,3,-*cd*]pyrene, 54.05 min; (8) bis(2-ethylhexyl)phthalate, 55.79 min; and (9) coronene, 68.12 min.

100 Fourier transform IR spectrometer and Starlab data system, a Hewlett-Packard (HP) 5890A capillary GC (Avondale, PA), and a Mattson Instruments matrix-isolation cryogenic module. The GC was equipped with an HP 19245A on-column injector, a flame ionization detector (FID), an HP 3392A integrator, and an HP 19405A sampler/event control unit.

The analytical column was a 30-m × 0.25-mm-i.d. DB-5 fused-silica capillary with a 0.25-μm film thickness (J & W. Scientific, Folsom, CA). The carrier gas was 0.62% argon in helium (National Welders, Raleigh, NC) and had a flow rate of 1.64 cm^3/min. The matrix-to-solute (M/S) ratio was estimated to be 1000 to 1 for a GC peak with a full width at half-height of 0.1 min containing 10 ng of a compound with a molecular weight of 228 daltons (e.g., benz[*a*]anthracene).

The effluent from the analytical column was split: 20% was directed to the FID and the remaining 80% was directed through an open-split cross,[19] then through a heated, fused-silica transfer line to the cryogenic disk. The splitter was made from a glass-lined union (Scientific Glass Engineering, Houston, TX) with a two-hole graphite/Vespel ferrule. The arms from the splitter were made from deactivated fused silica; a 30-cm length of 0.150-mm-i.d. tubing extended to the FID, and a 45-cm length of 0.250-mm-i.d. tubing extended to the open-split cross. The transfer line, a 60-cm length of 0.150-mm-i.d. deactivated fused silica, was enclosed in an insulated, heated stainless steel conduit.

The FID heating block, the transfer line conduit, and the deposition tip heating block were held at 300°C. The cryogenic disk was maintained at 14 K throughout matrix deposition and MI-IR spectral acquisition. The pressure in the cryogenic chamber was 2×10^{-4} Pa. The following GC temperature program was used: initial temperature of 40°C, hold for 4 min, increase at 20°C/min to 200°C, hold for 1 min, increase at 2°C/min to 300°C and hold for 10 min.

Single-beam sample spectra were ratioed to single-beam background spectra collected with the cryogenic disk positioned 0.30 min before the GC peak maximum and plotted as absorbance files. The MI-IR spectra were derived from 128 to 512 coadded, double-sided, 8192-point interferograms. A triangular apodization function and a zero-filling factor of 2 were applied to the coadded interferograms prior to the fast Fourier transform. This

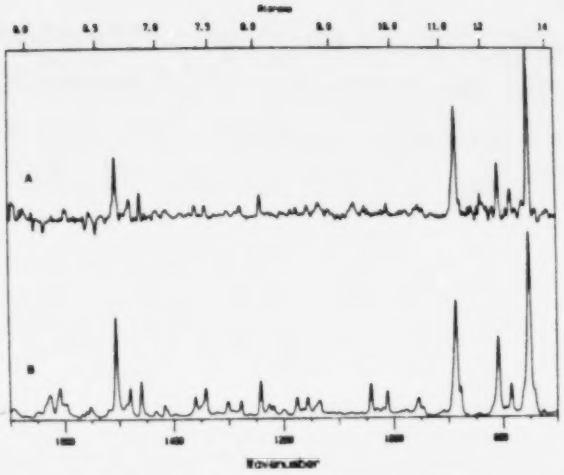

FIG. 2. MI-IR spectrum of (A) the component of the filter extract with a retention time of 31.24 min and (B) benz[*a*]anthracene reference standard.

resulted in MI-IR spectra with a nominal resolution of 4 cm^{-1}. Reference MI-IR spectra of PAH standards were also obtained at 4 cm^{-1} resolution and stored in an on-line spectral library. Additional MI-IR spectra of PAH standards were obtained at a nominal 2-cm^{-1} resolution for comparison to literature values of band maxima. All MI-IR spectra were baseline corrected.

The urban air particulate sample had been collected on an 8- × 10-in. quartz-fiber filter by a high-volume air sampler. An 8- × 1-in. portion of the filter was Soxhlet-extracted for 40 h with methylene chloride. The methylene chloride extract was concentrated and the solvent exchanged to cyclohexane. The extract was then fractionated on a silica gel column. The aromatic fraction of the extract was collected and concentrated by Kuderna-Danish evaporation.

RESULTS AND DISCUSSION

A portion of the GC/FID trace of the filter extract is shown in Fig. 1. Identifications of specific components in the filter extract were made by comparing their MI-IR spectra and retention times to those of authentic standards. The MI-IR spectrum of the first GC component of interest, which eluted at 31.24 min, is shown in Fig. 2A. This spectrum exhibited sharp spectral features, which are characteristic of MI-IR spectra, and an excellent signal-to-noise ratio. Although the concentrations of each component in the extract were not determined, the amount of the compound eluting at 31.24 min is estimated to be approximately 5 ng injected on-column. This corresponds to approximately 4 ng of the compound deposited onto the cryogenic disk. A computer-assisted search of the MI-IR spectral library identified this component as benz[*a*]anthracene (compare Fig. 2A and 2B).

The MI-IR spectrum of the GC peak that eluted at 31.58 min is shown in Fig. 3A. This spectrum exhibited band maxima at 817, 764, and 744 cm^{-1}. A search for this spectrum in the MI-IR spectral library did not yield an acceptable match. However, on the basis of its prox-

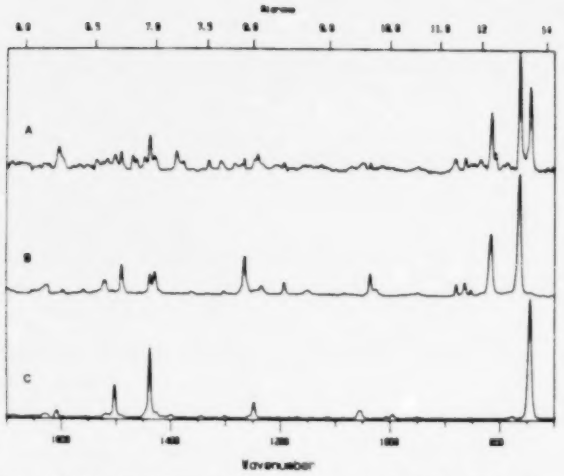

FIG. 3. MI-IR spectrum of (A) the component of the filter extract with a retention time of 31.58 min, (B) chrysene reference standard, and (C) triphenylene reference standard.

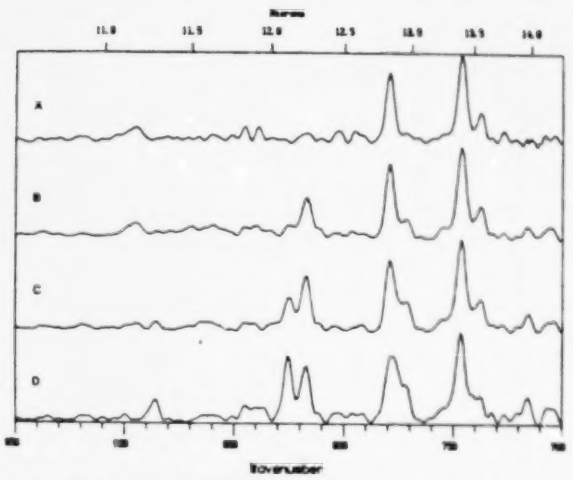

FIG. 5. MI-IR spectra of components of the filter extract with retention times of (A) 41.04, (B) 41.16, (C) 41.28, and (D) 41.46 min.

imity to the GC peak identified as benz[*a*]anthracene, this GC peak could be predicted to contain the chrysene-triphenylene isomer pair. Indeed, comparison of the spectrum in Fig. 3A to reference MI-IR spectra of chrysene (Fig. 3B) and triphenylene (Fig. 3C) clearly showed that spectral features characteristic of both isomers were present. The presence of chrysene was confirmed by subtracting a reference spectrum of triphenylene from the spectrum in Fig. 3A. A search for the subtraction result in the MI-IR reference library showed that chrysene was the best match (Fig. 4). Similarly, a reference spectrum of chrysene was subtracted from the spectrum in Fig. 3A, and triphenylene was found to be the best match in the library search (spectra not shown).

Chromatographic resolution of benz[*a*]anthracene and the chrysene-triphenylene isomer pair is not always achieved, and under most chromatographic conditions, chrysene and triphenylene co-elute. However, as shown above, each of these four-ring PAH isomers has a unique MI-IR spectrum and can be distinguished by GC/MI-IR spectrometry, even if it is not separated from the others chromatographically. This distinction is important because benz[*a*]anthracene and chrysene have been found to be carcinogens in animals, whereas triphenylene does not exhibit such carcinogenic activity.[3,4] In contrast, reference EI mass spectra of benz[*a*]anthracene, chrysene, and triphenylene all have a strong molecular ion at 228 daltons, have similar fragmentation patterns, and exhibit only subtle differences in the relative abundance of the fragmented ions.[20] Therefore, achieving a clear distinction between these isomers is difficult by EI-GC/MS alone.

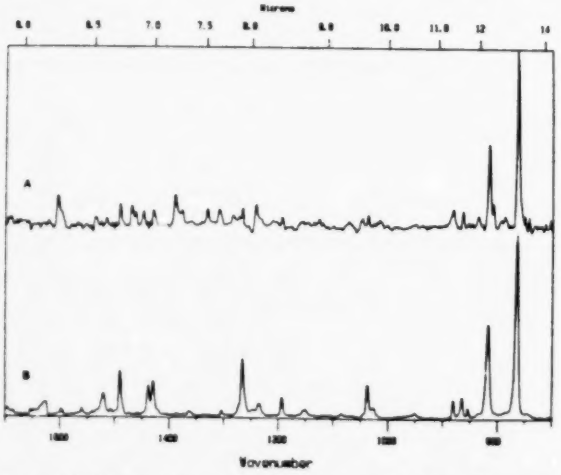

FIG. 4. MI-IR spectrum of (A) the component of the filter extract with a retention time of 31.58 min from which a reference MI-IR spectrum of triphenylene has been subtracted and (B) chrysene reference standard.

Another example of the ability of GC/MI-IR spectrometry to distinguish between isomeric PAHs is shown for the GC peak centered at 41.28 min, a retention time expected for the benzofluoranthene isomers. The GC peak at 41.28 min was relatively broad and appeared to be composed of more than one component. To determine whether this was the case, we acquired MI-IR spectra at discrete time intervals across the GC peak (Fig. 5). These spectra are plotted over the out-of-plane C-H bending region between 950 and 700 cm^{-1} to emphasize any differences between the co-eluting components. The MI-IR spectrum acquired at the leading edge of the peak (41.04 min) exhibited three bands at 779, 746, and 738 cm^{-1} (Fig. 5A). These bands were also present in the MI-IR spectrum at 41.16 min and were joined by two additional bands that appeared at 817 and 772 cm^{-1} (Fig. 5B). The MI-IR spectrum acquired at the GC peak maximum, 41.28 min, exhibited all of the bands observed in the previous scans, in addition to a band at 824 cm^{-1} (Fig. 5C). In the MI-IR spectrum obtained after the GC peak maximum, at 41.46 min, the band at 824 cm^{-1} increased in relative intensity, and an additional band at 886 cm^{-1} appeared. The band centered at 779 cm^{-1} also became broader (Fig. 5D).

The MI-IR spectra acquired at discrete time intervals across the GC peak centered at 41.28 min were compared to reference MI-IR spectra of the benzofluoranthene iso-

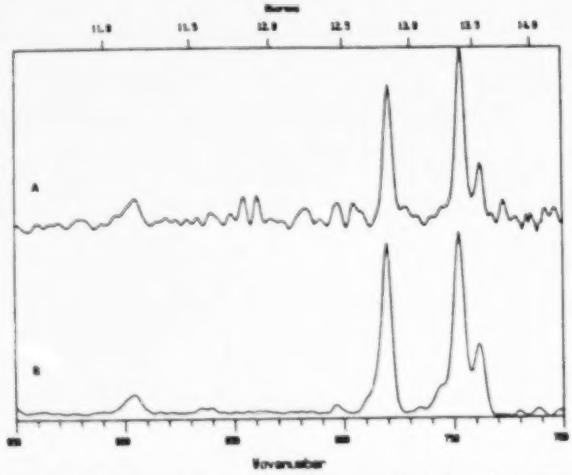

FIG. 6. MI-IR spectrum of (A) the component of the filter extract with a retention time of 41.04 min and (B) benzo[*b*]fluoranthene reference standard.

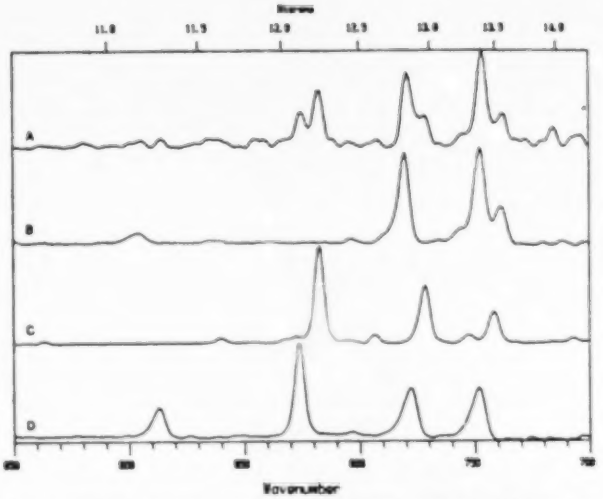

FIG. 8. MI-IR spectrum of (A) the component of the filter extract with a retention time of 41.28 min, (B) benzo[*b*]fluoranthene reference standard, (C) benzo[*j*]fluoranthene reference standard, and (D) benzo[*k*]fluoranthene reference standard.

mers. This comparison revealed the following: Benzo[*b*]fluoranthene was the only isomer present at the leading edge of the GC peak, 41.04 min (Fig. 6). Both the benzo[*b*]- and the benzo[*j*]fluoranthene isomers were present closer to the GC peak maximum, 41.16 min (Fig. 7). All three isomers, benzo[*b*]-, benzo[*j*]-, and benzo[*k*]fluoranthene, were present at the GC peak maximum, 41.28 min (Fig. 8). The relative amount of benzo[*k*]fluoranthene increased after the GC peak maximum (see Fig. 5D).

In this case, the three benzofluoranthene isomers, all of which are suspected or known carcinogens,[3,4] were unambiguously identified by GC/MI-IR spectrometry. In contrast, the EI mass spectra for these isomers all have a molecular ion at 252 daltons and exhibit nearly identical fragmentation patterns.[20] Therefore, once again, a distinction is made between PAH isomers that cannot easily be made by EI-GC/MS.

Benzo[*e*]pyrene and benzo[*a*]pyrene, isomeric PAHs with five fused rings, can also be distinguished by GC/MI-IR spectrometry. The unambiguous distinction between these isomers is important because benzo[*a*]pyrene is a potent carcinogen, whereas benzo[*e*]pyrene has only slight carcinogenic activity.[3,4] The GC/FID trace for the filter extract exhibited a triplet of unresolved peaks between 43 and 44 min (see Fig. 1), which is the region of the chromatogram where the benzopyrene isomers are expected to elute. An MI-IR spectrum acquired at 43.61 min exhibited bands that are characteristic of benzo[*e*]pyrene, but also contained additional bands. The spectral features due to benzo[*e*]pyrene were brought out by subtracting an MI-IR spectrum acquired at 43.78 min from one acquired at

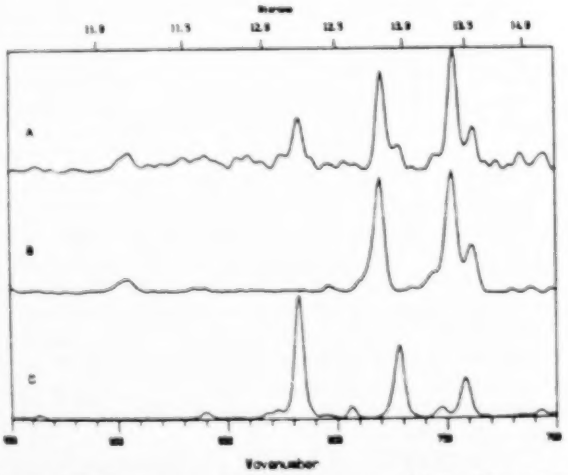

FIG. 7. MI-IR spectrum of (A) the component of the filter extract with retention time of 41.16 min, (B) benzo[*b*]fluoranthene reference standard, and (C) benzo[*j*]fluoranthene reference standard.

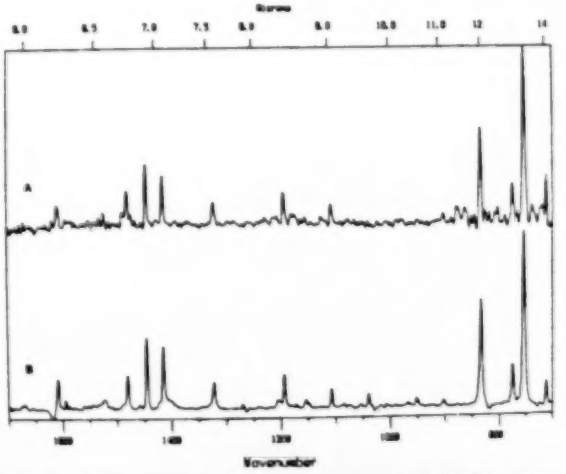

FIG. 9. MI-IR spectrum of (A) the component of the filter extract with a retention time of 43.61 min from which an MI-IR spectrum acquired at 43.78 min has been subtracted and (B) benzo[*e*]pyrene reference standard.

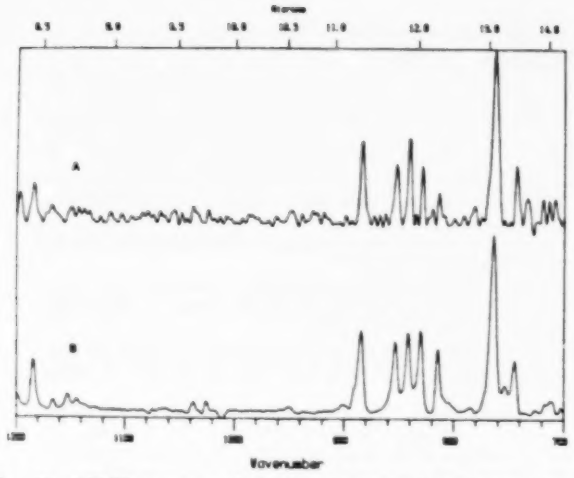

FIG. 10. MI-IR spectrum of (A) the component of the filter extract with a retention time of 44.03 min and (B) benzo[*a*]pyrene reference standard.

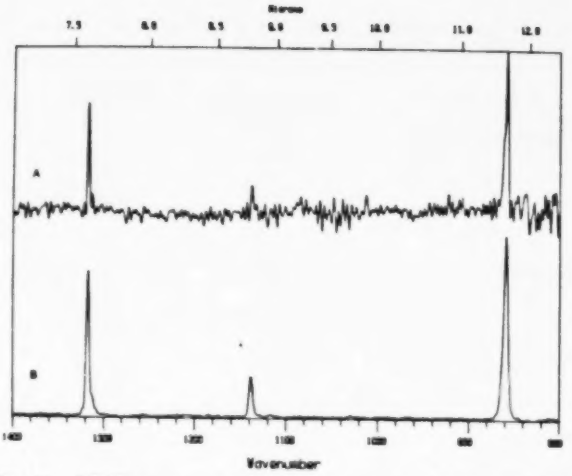

FIG. 11. MI-IR spectrum of (A) the component of the filter extract with a retention time of 68.12 min and (B) coronene reference standard.

43.61 min. A search for the subtraction result (Fig. 9A) in the reference MI-IR spectral library confirmed the identity of the GC peak at 43.61 min as benzo[*e*]pyrene (compare Fig. 9A and 9B). The MI-IR spectrum acquired at 44.03 min was identified as benzo[*a*]pyrene by a search of the reference MI-IR spectral library (Fig. 10). In this case, no spectral subtraction was needed. In the same way, the component that eluted at 44.79 min was identified as perylene, another five-ring PAH isomer (spectra not shown). It is noteworthy that, although benzo[*e*]pyrene, benzo[*a*]pyrene, and perylene were separated chromatographically, these isomers can also be distinguished by their MI-IR spectra. Again, an unambiguous assignment of these isomers cannot be made on the basis of only their mass spectra and retention times. In fact, the EI mass spectra of benzo[*e*]pyrene, benzo[*a*]pyrene, and perylene are virtually identical to the EI mass spectra of the benzofluoranthene isomers.[20]

One other capability that GC/MI-IR spectrometry provides is the ability to analyze PAHs with relatively high boiling points. Most conventional, light-pipe-based GC/IR systems are limited in the analysis of these compounds by the inverse relationship between the IR signal intensity and the operating temperature of the interface.[21] Although this effect has been significantly reduced in a prototype system,[22] most light-pipe-based GC/IR systems suffer from this problem. For instance, a one-third loss in signal intensity was recently reported for a state-of-the-art commercial GC/IR system, which was being evaluated for environmental analyses, when the light-pipe temperature was raised from 25 to 300°C.[5] However, in GC/MI-IR, the separation and detection of components in a mixture are independent steps. This allows conditions for the chromatography and the spectrometry to be optimized without compromising one or the other. Therefore, the interface between the GC and the cryogenic module can be operated at a relatively high temperature, such as 300°C, which permits the analysis of PAHs with high boiling points. For example, the component eluting at 54.05 min was identified as indeno[1,2,3-*cd*]pyrene, a six-ring carcinogenic PAH, by searching for a match of its MI-IR spectrum in the MI-IR spectral library (spectra not shown). Likewise, the MI-IR spectrum of the component eluting at 68.12 min was identified as coronene, a seven-ring PAH with a boiling point of 525°C (see Fig. 11).

As mentioned previously, MI-IR spectrometry has been used extensively to characterize PAHs.[6-11] Except for preliminary experiments illustrating the combination of GC and MI-IR spectrometry,[11] conventional slow-spray-on (SSO) techniques, which often require between 1 and 2 h of total deposition time,[6] were used for matrix deposition. One concern in GC/MI-IR spectrometry is whether adequate matrix isolation is achieved under the rapid sample deposition conditions that are necessary in order to maintain the chromatographic resolution of the individual, separated components. This topic has been examined in detail for a variety of compound classes (see Ref. 23 and references therein). In light of this concern, GC/MI-IR data were obtained for PAHs over a concentration range of 5 to 100 ng injected on-column (M/S ratio ranging from approximately 2000:1 to 100:1) and compared to data obtained previously by using SSO deposition (see Table I).[7,24] The IR band maxima and half-bandwidths obtained under GC/MI-IR conditions (with 2-cm^{-1} resolution) for selected PAHs were constant over this concentration range and are similar to those obtained by using SSO deposition. Most values for the band maxima agree to within 1 to 4 cm^{-1}, with the worst discrepancy being 5 cm^{-1}. The half-bandwidths for the IR bands measured under GC/MI-IR conditions are comparable to the maximum half-bandwidths, which ranged from 4 to 8 cm^{-1}, measured under SSO conditions with an M/S ratio of 1000:1. However, when a higher M/S ratio (5×10^4:1) was used for SSO deposition, the half-bandwidths decreased to between 1 and 3 cm^{-1} and singlets were resolved into doublets.[7] Unfortunately, high M/S ratios are unachievable in the GC/MI-IR experiment because the matrix does not adhere to the cryogenic disk if the matrix becomes too thick. Under the experimental conditions used in this study, this occurs when

TABLE I. IR band maxima (cm^{-1}) for selected PAHs obtained by slow-spray-on (SSO)[7,24] and GC/MI-IR deposition.

Compound	SSO deposition	GC/MI-IR deposition
Benz[a]anthracene	1504	1504
	1365	1360
	886	883
	809	805
	785	783
	752	748
Chrysene	1365	1364
	1234	...
	(819, 816)	813
	765	762
Triphenylene	1502	1501
	1438	1438
	746	742
Perylene	1498	1500
	1385	1385
	818	816
	(776, 774)	772
Benzo[a]pyrene	1184	1183
	(888, 886)	882
	855	852
	843	840
	831	828
	765	762
	747	742
	694	692
Benzo[e]pyrene	1480	1479
	1444	1445
	1415	1414
	883	...
	(755, 753)	750

the percentage of argon in the carrier gas approaches 2% (or a M/S ratio greater than 3000:1 for 10 ng of benz[a]anthracene injected on-column).

Also, it is well documented that the matrix itself exerts an influence on the appearance of MI-IR spectra.[25-27] Often the use of different matrix gases results in the formation of different trapping sites within the matrix, which can cause band-splitting and shifts in absorption maxima. These effects might account for the subtle differences observed in the MI-IR spectra obtained under GC/MI-IR conditions (with an argon matrix) compared to those obtained under SSO conditions (with a nitrogen matrix).

CONCLUSIONS

This study shows that GC/MI-IR spectrometry has the sensitivity to detect PAHs in fractionated extracts of urban air particulate matter and the molecular specificity to discriminate between PAH isomers, even when they are not separated chromatographically. By the use of GC/MI-IR spectrometry, isomeric PAHs that exhibit different biological activities, but are difficult to distinguish by EI-GC/MS, can be unambiguously identified. GC/MI-IR spectrometry is certainly a viable technique for the qualitative analysis of PAHs and other organic compounds in air sample extracts. Current activities in our laboratory are focused on investigating the potential of GC/MI-IR spectrometry for the quantitative analysis of PAHs and other semivolatile organic compounds in environmental samples.

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